A FINITE ELEMENT METHOD FOR REACTION-DIFFUSION SYSTEMS ON GROWING DOMAINS

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ABSTRACT. We present a finite element method for the approximation of semilinear reaction-diffusion systems on growing domains. We prove optimal error estimates in the $L^2$ norm. We conduct numerical experiments that support the theoretical results and that demonstrate novel solution behaviour of Turing-type reaction-diffusion systems on growing two-dimensional domains.

1. INTRODUCTION

Since the seminal work of Turing, A. M. [30] reaction-diffusion systems (RDSs) have been proposed as the underlying mechanism behind many pattern formation phenomena in developmental biology. Formation of patterns occurs mostly during the growth phase of organisms, and in many cases the growth itself is what causes the patterns to appear and evolve [24]. Numerical simulations of RDSs on growing or evolving domains reproducing empirically observed pattern formation processes abound in the literature [3, 4, 14, 23]. The analysis of such schemes to approximate the solution to RDSs on fixed or evolving domains is thus an important and active area of research.

On fixed domains, Zhang et al. [35] analyse a second order implicit-explicit finite element scheme for the Gray-Scott model and Garvie and Trenchea [11] analyse a first order scheme for an RDS that models predator prey dynamics. Recently Mackenzie and Madzvamuse [17] analysed a finite difference scheme approximating the solution of a linear RDS on a domain with continuous spatially linear isotropic evolution. Our study is novel, in that, we propose and analyse a finite element method to approximate RDSs on a domain with continuous (possibly nonlinear) evolution. The finite element method is robust for the applications we have in mind, as the problems are often posed on complex geometries such as the surface of an organism. We assume prescribed domain evolution and we derive corresponding finite element formulations via the Eulerian and the Lagrangian frameworks, common in fluid dynamics. To deal with the nonlinear reaction kinetics, we make some assumptions on the regularity of the continuous problem guided by our theoretical results published in Venkataraman et al. [32]. Although our work is motivated by applications relating to biological pattern formation, we formulate the scheme with abstract reaction kinetics and domain evolution, so that the analysis is applicable to similar mathematical problems in other fields. For simplicity we restrict our discussion to the case where both the reference domain and the evolving domain are flat. We reconcile the theoretical error analysis of the scheme with a series of numerical results; that exhibit novel solution behaviour of 2 or 3 component reaction diffusion systems on continuously evolving domains. In another study [33], we show that the Eulerian form of the method is applicable the approximation of an RDS posed on an evolving surface.

The layout of the remainder of this discussion is as follows: In §2 we introduce our notation, we state our model problem together with the assumptions that we make on the problem data and the domain evolution. We present the weak formulation of the continuous problem and define a modified nonlinear reaction function which we introduce for the analysis. In §3 we present the semidiscrete (space-discrete) and fully discrete finite element schemes, we analyse both schemes proving optimal (order) convergence rates. We also derive a stability result in the semidiscrete case, whereby the stabilising effect of domain

Date: 23rd November 2011.
growth observed in the continuous case is preserved. In \[\S4\] we provide a concrete implementation of the finite element scheme with a set of reaction kinetics commonly encountered in developmental biology, considering domains with spatially linear and nonlinear evolution. In \[\S5\] we perform some numerical experiments to illustrate our theoretical results and to study as yet unexplored solution behaviour exhibited by RDSs on evolving domains in 2 space dimensions. Finally, in \[\S6\] we summarise our results, draw conclusions and indicate possible directions for future research.

2. Notation and Setup

2.1. Calculus and function spaces. Given an open and bounded domain \(\Pi \subset \mathbb{R}^d\) and a function \(\eta \in C^1(\Pi; \mathbb{R}^m)\), we define the Jacobian matrix of \(\eta\)

\[
\nabla \eta(x) := \begin{bmatrix}
\frac{\partial \eta_1}{\partial x_1}(x) & \cdots & \frac{\partial \eta_m}{\partial x_1}(x) \\
\vdots & \ddots & \vdots \\
\frac{\partial \eta_1}{\partial x_d}(x) & \cdots & \frac{\partial \eta_m}{\partial x_d}(x)
\end{bmatrix}, \text{ for } x \in \Pi,
\]

and the divergence of \(\eta\)

\[
\nabla \cdot \eta(x) := \sum_{i=1}^d \frac{\partial \eta_i}{\partial x_i}(x).
\]

For the case of a scalar-valued function \(\eta \in C^1(\Pi; \mathbb{R})\), we define the Laplacian of \(\eta\)

\[
\Delta \eta(x) := \sum_{i=1}^d \frac{\partial^2 \eta}{\partial x_i^2}(x).
\]

In an effort to compress notation for spatial derivatives, we introduce the convention used above, that if the variable with respect to which we differentiate is omitted, it should be understood as the spatial argument of the function.

We denote by \(L^p(\Pi)\), \(W^{p,k}(\Pi)\) and \(H^k(\Pi)\) the Lebesgue, Sobolev and Hilbert spaces respectively, as defined by the following: for measurable \(\eta\) and for \(p, k \in [1, \infty)\)

\[
L^p(\Pi) := \left\{ \eta : \int_{\Pi} |\eta|^p < \infty \right\},
\]

\[
L_\infty(\Pi) := \left\{ \eta : \sup_{x \in \Pi} |\eta(x)| < \infty \right\},
\]

\[
W^{p,k}(\Pi) := \left\{ \eta \in L^p(\Pi) : \sum_{\alpha \leq k} \nabla^\alpha \eta \in L^p(\Pi) \right\},
\]

\[
H^k(\Pi) := W^{2,k}(\Pi).
\]

For measurable functions \(\eta, \mu : \Pi \to \mathbb{R}\), we introduce the following notation

\[
\langle \eta, \mu \rangle_\Pi := \int_{\Pi} \eta(x) \mu(x) \, dx,
\]

\[
\|\eta\|_{L^2(\Pi)} := \langle \eta, \eta \rangle_{\Pi}^{1/2},
\]

\[
|\eta|_{H^k(\Pi)} := \left\| \nabla^k \eta \right\|_{L^2(\Pi)}, \text{ for } k \in \mathbb{Z}_+,
\]

\[
\|\eta\|_{H^k(\Pi)} := \left( \|\eta\|_{L^2(\Pi)}^2 + \sum_{j=1}^k |\eta|_{H^j(\Pi)}^2 \right)^{1/2}.
\]
For vector valued functions $\eta, \mu : \Omega \rightarrow \mathbb{R}^m$, we denote
\[(\eta, \mu)_{\Omega,m} := \sum_{i=1}^{m} \int_{\Omega} \eta_i(x)\mu_i(x) \, dx,\]
with the corresponding modifications to the norms and seminorms.

2.2. Evolving domains. Let $\{\Omega_t : 0 \leq t \leq T\}$ be a simply connected family of evolving time-dependent domains, and let $\hat{\Omega}$ be a simply connected time-independent reference domain with Lipschitz boundary. Throughout this study we assume domain evolution is known and that there exists a “smooth”\footnote{We shall formalise this assumption in the proceeding sections.} one to one mapping between the reference and evolving domains. We assume there exists a time-differentiable family of $C^1$-diffeomorphisms $A : \hat{\Omega} \times [0, T] \rightarrow \Omega_t$ such that at each instant $t \in [0, T]$ and for each $x \in \Omega_t$ there exists a $\xi \in \hat{\Omega}$ such that
\[
A(\xi, t) = x.
\]
The Jacobian $J$ of the diffeomorphism $A(\cdot, t)$ with respect to the spatial (reference) variable and its determinant $J$ are given by
\[
J(\xi, t) := \nabla A(\xi, t) \quad \text{and} \quad J(\xi, t) := \det J(\xi, t) \quad \xi, t \in \hat{\Omega} \times [0, T].
\]
Furthermore we will denote by $K$
\[
K(\xi, t) := \nabla A^{-1}(A(\xi, t)) \quad \xi, t \in \hat{\Omega} \times [0, T].
\]
We denote by $a$
\[
a(x, t) := \partial_2 A(A(x, t), t) \quad \text{for } x \in \Omega_t \text{ and } t \in [0, T].
\]
From classical results \cite{1} we have the following expression
\[
\partial_t J(\xi, t) = J(\xi, t) \nabla \cdot a(A(\xi, t), t) \quad \xi, t \in \hat{\Omega} \times [0, T].
\]
To aid the exposition we define $Q$ to be the topologically cylindrical space-time domain:
\[
Q := \{(x, t) : x \in \Omega_t, t \in [0, T]\}.
\]
We now introduce notation to relate functions defined on the evolving domain to functions defined on the reference domain. Given a function $g : Q \rightarrow \mathbb{R}$ we denote by $\hat{g} : \hat{\Omega} \times [0, T] \rightarrow \mathbb{R}$ its pullback on the reference domain, defined by the following relationship
\[
\hat{g}(\xi, t) := g(A(\xi, t), t) \quad \xi, t \in \hat{\Omega} \times [0, T].
\]
Assuming sufficient smoothness on the function $g$, using (2.19) and the chain rule we may relate time-differentiation on the reference and evolving domains:
\[
\partial_t \hat{g}(\xi, t) = \partial_t g(A(\xi, t), t) + [a \cdot \nabla g](A(\xi, t), t) \quad \xi, t \in \hat{\Omega} \times [0, T].
\]
The right hand side of (2.20) is commonly known as the material derivative of $g$ with respect to the motion $A$. The following result relates the norm of a function $g : Q \rightarrow \mathbb{R}$ on the evolving domain with its pullback $\hat{g}$ on the reference domain:
\[
\|g\|_{L^2(Q_t)}^2 = \langle J \hat{g}, \hat{g} \rangle_{\hat{\Omega}}.
\]
For the gradient of a function of a sufficiently smooth function $g : Q \rightarrow \mathbb{R}$, we have
\[
\|\nabla g\|_{L^2(Q_t)}^2 = \langle JK \nabla \hat{g}, K \nabla \hat{g} \rangle_{\hat{\Omega}}.
\]
We now present the model equation we wish to consider, an RDS posed on a continuously deforming domain. Our model takes the form of a system of chemicals that are coupled only through the reaction terms and diffuse independently of each other. Given an integer $m \geq 1$, Let $u(x, t)$ be an $(m \times 1)$
vector of concentrations of chemical species, with \( x \in \Omega_t \subset \mathbb{R}^d, \ d = 1, 2, 3, \) the spatial variable and \( t \in [0, T], \ T > 0, \) the time variable. The model we shall consider is of the following form (see \cite{19} for details of the derivations):

2.3. **Problem** (RDS on a time-dependent domain). Find \( u_i, \) functions from \( \Omega_t \) into \( \mathbb{R}, \) such that for \( i = 1, \ldots, m, \) \( u_i \) satisfies

\[
\begin{align*}
\partial_t u_i(x, t) - D_i \Delta u_i(x, t) + \nabla \cdot [a \nabla u_i](x, t) &= f_i(u(x, t)), \quad x \in \Omega_t, t \in (0, T], \\
[\nu \cdot \nabla u_i](x, t) &= 0, \quad x \in \partial \Omega_t, t > 0, \\
u_i(x, 0) &= u_i^0(x), \quad x \in \Omega_0,
\end{align*}
\]

(2.23)

where \( \Omega_t \) is a simply connected bounded continuously deforming domain with respect to \( t, \) with Lipschitz boundary \( \partial \Omega_t \) at time \( t \in [0, T]. \) The vector of nonlinear coupling terms \( f := (f_1, \ldots, f_m)^T \) is assumed to be locally Lipschitz-continuous, \( D := (D_1, \ldots, D_m)^T \) is a vector of strictly positive diffusion coefficients, \( a = (a_1, \ldots, a_d)^T \) is a flow velocity generated by the evolution of the domain and the initial data \( u_0(x) \) is bounded vector valued function.

2.4. **Assumption** (Bounded solutions and classically differentiable reaction function). We assume, \( u \) the solution of Problem (2.23), to be bounded for all \( t \in [0, T]. \) For \( i = 1, \ldots, m, \) we define

\[
\begin{align*}
u_i^- := \inf_{Q} u_i, \\
u_i^+ := \sup_{Q} u_i,
\end{align*}
\]

(2.24)

and denote by \( I_u := \Pi_{i=1}^m [\nu_i^-, \nu_i^+] \subset \mathbb{R}^m \) the range of \( u. \) We assume that for some fixed \( \delta \in \mathbb{R}^+, \) the nonlinear reaction function \( f \) belongs to \( C^1(I_\delta), \) where we denote by \( I_\delta \) the closed set

(2.25)

\[
\prod_{i=1}^m [\nu_i^- - \delta, \nu_i^+ + \delta].
\]

2.5. **Remark** (Applicability of Assumption 2.4). In Venkataraman et al. \cite{32}, we proved the global existence of positive classical solutions to Problem (2.23) for a class of RDSs with positive initial data on domains with bounded spatially linear isotropic evolution. In this case, if \( f \) belongs to \( C^1(\mathbb{R}^m), \) Assumption 2.4 holds with the region \( I_\delta \) a subset of \( \mathbb{R}^m. \)

2.6. **Assumption** (Regularity of the mapping). We assume the following regularity on the mapping \( \mathcal{A} \) between the the reference domain \( \hat{\Omega} \) and the evolving domain \( \Omega_t : \)

\[
\mathcal{A} \in C^{k+1}(\hat{\Omega}) \cap C^1(0, T),
\]

(2.26)

where \( k \) will be taken equal to the degree of the basis functions of the finite element space defined in the following section. To ensure the mapping is invertible we assume the determinant of the Jacobian \( J \) of the mapping \( \mathcal{A} \) (cf. 2.14) satisfies

(2.27)

\[
J > 0 \text{ in } \hat{\Omega} \times [0, T].
\]

2.7. **Remark** (Regularity under the mapping). Classical results \cite{32} Th. 3.41] allow us to relate regularity on the evolving domain to regularity on the reference domain. Let Assumption 2.6 hold. For a function \( g : \hat{Q} \to \mathbb{R} \) with the corresponding function on the reference domain \( \hat{g} : \Omega \times [0, T] \to \mathbb{R} \) defined by \( \mathcal{A}, \) we have for \( p \geq 1 \) and \( t = 0, \ldots, k + 1, \)

\[
v \in L_p \left( 0, T; H^k(\Omega_t) \right) \iff \hat{v} \in L_p \left( 0, T; H^k(\hat{\Omega}) \right),
\]

(2.28)

\[
\partial_t v \in L_p \left( 0, T; H^{k+1}(\Omega_t) \right) \iff \partial_t \hat{v} \in L_p \left( 0, T; H^{k+1}(\hat{\Omega}) \right).
\]

(2.29)
2.8. **Remark** (Sufficient but not necessary regularity). For the applications we have in mind the domain velocity is prescribed and Assumption 2.6 is valid. Deriving minimal assumptions on the regularity of the mapping is not the focus of this study. Formaggia and Nobile [10] Pr. 2.1 show that a necessary and sufficient condition for the regularity result (2.28) with \( k = 0 \) is

\[
J > 0, \mathcal{A} \in W^{1,\infty}(\hat{\Omega}) \text{ and } \mathcal{A}^{-1}(\cdot, t) \in W^{1,\infty}(\Omega_t) \text{ for } t \in [0, T].
\]

Minimal regularity assumptions would be important if the mapping was determined by the finite element functions. For example, scenarios we wish to consider in future studies are the case of concentration driven domain evolution or the case where evolution of the boundary curve of the domain alone is prescribed and the internal nodes are moved according to principles of elasticity.

2.9. **Weak formulations.** For the purposes of constructing a finite element discretisation, we introduce a weak formulation associated with Problem (2.23). The problem is to find \( u_i \in L_2 \left(0, T; H^1(\Omega_t)\right) \) with \( \partial_t \hat{u}_i \in L_2 \left(0, T; H^{-1}(\Omega_t)\right) \) such that for each \( i = 1, \ldots, m \)

\[
\langle \partial_t u_i + \nabla \cdot (a u_i), \chi \rangle_{\Omega_t} + \langle D_i \nabla u_i, \nabla \chi \rangle_{\Omega_t} = \langle f_i(u), \chi \rangle_{\Omega_t}, \quad \forall \chi \in H^1(\Omega_t).
\]

We use (2.20) and (2.28) to write an equivalent formulation on the reference domain \( \hat{\Omega} \). Find \( \hat{u}_i \in L_2 \left(0, T; H^1(\hat{\Omega})\right) \) with \( \partial_t \hat{u}_i \in L_2 \left(0, T; H^{-1}(\hat{\Omega})\right) \) such that

\[
\langle \partial_t \hat{u}_i + \hat{u}_i \nabla \cdot (a(\hat{\xi}, t)), \hat{\chi} \rangle_{\hat{\Omega}} + \langle D_i \nabla \hat{u}_i, K \nabla \hat{\chi} \rangle_{\hat{\Omega}} = \langle J f_i(u), \hat{\chi} \rangle_{\hat{\Omega}},
\]

for all \( \hat{\chi} \in H^1(\hat{\Omega}) \). Using the expression for the time-derivative of the determinant of the Jacobian (2.17), we have

\[
\langle \partial_t (J \hat{u}_i), \hat{\chi} \rangle_{\hat{\Omega}} + \langle D_i J K \nabla \hat{u}_i, K \nabla \hat{\chi} \rangle_{\hat{\Omega}} = \langle J f_i(u), \hat{\chi} \rangle_{\hat{\Omega}}, \quad \forall \hat{\chi} \in H^1(\hat{\Omega}).
\]

We shall use (2.33) to construct a finite element scheme to approximate the solution to Problem (2.23) on the reference domain. In [1] we illustrate that the resultant scheme may be solved on the reference or the evolving domain. We now define a further weak formulation on the evolving domain. We assume the test functions \( \hat{\chi} \in H^1(\hat{\Omega}) \) are time-independent. Therefore due to the regularity of the mapping (2.28) and the relationship between time-differentiation on the reference and evolving domains (2.20), \( \hat{\chi} \in H^1(\Omega_t) \) and \( \partial_t \hat{\chi} \in L_2 (\Omega_t) \). We thus obtain the following weak formulation on \( \Omega_t \), find \( u_i \in L_2 \left(0, T; H^1(\Omega_t)\right) \)

with \( \partial_t u_i \in L_2 \left(0, T; H^{-1}(\Omega_t)\right) \) such that

\[
\frac{d}{dt} \langle u_i, \chi \rangle_{\Omega_t} - \langle u_i, \partial_t \chi + a \cdot \nabla \chi \rangle_{\Omega_t} + \langle D_i \nabla u_i, \nabla \chi \rangle_{\Omega_t} = \langle f_i(u), \chi \rangle_{\Omega_t}, \quad \forall \chi \in H^1(\Omega_t) \text{ and } \partial_t \chi \in L_2 (\Omega_t).
\]

2.10. **Modified nonlinear reaction function.** In general the techniques used to show Assumption 2.4 holds utilise the maximum principle [28,32]. In the discrete case, the absence of a maximum principle [29 pg. 83] means we cannot guarantee the discrete solution remains in the region \( I_0 \). For the purposes of our analysis we introduce a modified *globally Lipschitz* nonlinear reaction function. Recalling \( I_0 \) from Assumption 2.4, we define \( \tilde{f} \in C^1(\mathbb{R}^m) \) such that

\[
\begin{cases}
\tilde{f}(z) = f(z), & \text{for } z \in I_0, \\
|\tilde{f}'(z)| < \tilde{C}, & \text{for } z \in \mathbb{R}^m.
\end{cases}
\]

The function \( \tilde{f} \) exists due to Assumption 2.4 (an extension of \( f \) with constant gradient outside \( I_0 \) suffices). We note that due to Assumption 2.4 if \( u \) is a solution of (2.23)

\[
\tilde{f}(u) = f(u).
\]
Thus, we may without restriction replace \( f \) with \( \tilde{f} \) in (2.23).

### 3. Finite element method

We shall split the spatial and temporal discretisation of Problem (2.23) into separate steps. For the spatial approximation, we employ a conforming finite element method. To this end, we define \( \hat{T} \) a triangulation of the reference domain. We shall consistently denote by \( h := \max_{s \in \hat{T}} \text{diam}(s) \) the mesh-size of \( \hat{T} \). We assume the triangulation \( \hat{T} \) fulfills the following properties:

- By \( s \in \hat{T} \) we mean \( s \) is an open simplex (interval, triangle or tetrahedron for \( d = 1, 2 \) or 3 respectively).
- \( \hat{T} \) is conforming, i.e., for any \( s, k \in \hat{T} \), \( s \cap k \) is either \( \emptyset \), a vertex, an edge or a face common to \( s \) and \( k \) or the full simplex \( s = k \).
- No error due to boundary approximation, i.e., \( \cup_{s \in \hat{T}} \partial s = \bar{\Omega} \) (we make this assumption for ease of exposition and it may be relaxed depending on the applications in mind).

For a sequence \( \{ \hat{T} \}_i \) of conforming triangulations, we assume the quasi-uniformity of the sequence holds, i.e., there exist \( C_1, C_2 \) independent of \( i \) such that

\[
C_1 h \leq \hat{h}_s \leq C_2 \hat{h}_s^2, \quad \text{for all} \ s \in \hat{T}, \ i = 1, 2, \ldots,
\]

where \( \hat{h}_s \) and \( \hat{h}_s \) are the radius of the largest ball contained in \( s \) and the diameter of \( s \) respectively.

Furthermore we note that our assumption of quasi-uniformity implies that the family of triangulations is shape-regular \([27] \text{ pg. 159}]\).

Given the triangulation \( \hat{T} \), we now define a finite element space on the reference configuration:

\[
V := \left\{ \hat{\Phi} \in H^1(\bar{\Omega}) : \hat{\Phi}|_s \text{ is piecewise polynomial of degree } \ell \right\}.
\]

We utilise the following known results about the accuracy of the finite element space \( V \). By the definition of \( V \), we have for \( \hat{v} \in H^{\ell+1}(\bar{\Omega}) \) (see for example Brezzi and Scott \([6] \text{ or Thomée }[29] \))

\[
\inf_{\hat{\Phi} \in V} \left\{ \| \hat{v} - \hat{\Phi} \|_{L^2(\bar{\Omega})} + \hat{h} \| \nabla (\hat{v} - \hat{\Phi}) \|_{L^2(\bar{\Omega})} \right\} \leq C h^{\ell+1} |\hat{v}|_{H^{\ell+1}(\bar{\Omega})}.
\]

In the analysis we shall make use of the fact that (3.3) is satisfied by taking the Lagrange interpolant \( \Lambda^h \hat{\Phi} : H^{\ell+1}(\bar{\Omega}) \to V \) in place of \( \hat{\Phi} \). Let \( \mathcal{I} : C^0 \to V \) be a Clément type interpolant \([7] \) and \( \ell + 1 > \frac{d}{2} \), where \( d \) is the spatial dimension. The following bound holds

\[
\| \hat{v} - \mathcal{I}^h \hat{\Phi} \|_{L^\infty(\bar{\Omega})} \leq C h^{\ell+1-d/2} |\hat{v}|_{H^{\ell+1}(\bar{\Omega})}.
\]

We shall make use of the following inverse estimate valid on quasiuniform sequences of triangulations:

\[
\| \hat{\Phi} \|_{L^\infty(\bar{\Omega})} \leq C h^{-d/2} \| \hat{\Phi} \|_{L^2(\bar{\Omega})} \quad \forall \hat{\Phi} \in \hat{V},
\]

where \( d \) is the spatial dimension.

#### 3.1. Semidiscrete approximation.**

We define the semidiscrete approximation (space-discrete) to the solution of Problem (2.23) to be a function \( \hat{u}^h : [0, T] \to \hat{V} \), such that for \( i = 1, \ldots, m \),

\[
\begin{cases}
\langle \partial_t (J \hat{u}_i^h), \hat{\Phi} \rangle_{\bar{\Omega}} + \langle D_i J K \nabla \hat{u}_i^h, K \nabla \hat{\Phi} \rangle_{\bar{\Omega}} = \langle J \tilde{f}_i(\hat{u}^h), \hat{\Phi} \rangle_{\bar{\Omega}} \quad \forall \hat{\Phi} \in \hat{V}, \\
\hat{u}_i^h(0) = \Lambda^h \hat{u}_i^0,
\end{cases}
\]

where \( \Lambda^h \) is the Lagrange interpolant.

#### 3.2. Proposition (Solvability of the semidiscrete scheme). Let Assumptions 2.4 and 2.6 hold. Then, the semidiscrete scheme (3.6) possesses a unique solution \( \hat{u}^h \in L^\infty(0, T)^m \).
Proof. In (3.6) if we write \( \hat{u}_i^h(t) \) as \( \sum_{j=1}^{\dim(\hat{V})} \alpha_j \hat{\Phi}_j \), we obtain a system of \( \dim(\hat{V}) \) ordinary differential equations for each \( i \). By assumption the initial data for each ODE is bounded. From Assumption 2.6 and the construction of \( \hat{f} \), we have that \( J, \hat{f}, f \) and their product are continuous globally Lipschitz functions. From ODE theory (for example [25]) we conclude that (3.6) possesses a unique bounded solution.

3.3. The effect of domain evolution on the semidiscrete solution. We now examine the stability of (3.6) and show that domain growth has a diluting or stabilising effect on the semidiscrete solution, mirroring results for the continuous problem [15]. Taking \( \dot{\hat{u}}_i^h \) in (3.6) gives for \( i = 1, \ldots, m, \)

\[
\left\langle \partial_t (J \hat{u}_i^h), \hat{u}_i^h \right\rangle_{\hat{\Omega}} + \left\langle D_i J K \nabla \hat{u}_i^h, K \nabla \hat{u}_i^h \right\rangle_{\hat{\Omega}} = \left\langle J \hat{f}_i(\hat{u}^h), \hat{u}_i^h \right\rangle_{\hat{\Omega}}.
\]

For the first term on the left of (3.7) we have

\[
\left\langle \partial_t (J \hat{u}_i^h), \hat{u}_i^h \right\rangle_{\hat{\Omega}} = \frac{d}{dt} \left\langle J \hat{u}_i^h, \hat{u}_i^h \right\rangle_{\hat{\Omega}} - \left\langle J \hat{u}_i^h, \partial_t \hat{u}_i^h \right\rangle_{\hat{\Omega}}.
\]

Using (2.19) and (2.20) we have

\[
\left\langle \partial_t (J \hat{u}_i^h), \hat{u}_i^h \right\rangle_{\hat{\Omega}} = \frac{d}{dt} \left\langle \hat{u}_i^h, \hat{u}_i^h \right\rangle_{\hat{\Omega}} - \left\langle \hat{u}_i^h, \partial_t \hat{u}_i^h + a \cdot \nabla \hat{u}_i^h \right\rangle_{\hat{\Omega}}.
\]


\[
\left\langle \partial_t (J \hat{u}_i^h), \hat{u}_i^h \right\rangle_{\hat{\Omega}} = \frac{1}{2} \left( \frac{d}{dt} \left\langle \hat{u}_i^h, \hat{u}_i^h \right\rangle_{\hat{\Omega}} + \left\langle \hat{u}_i^h, \hat{u}_i^h \cdot \nabla a \right\rangle_{\hat{\Omega}} \right).
\]

Now dealing with the right hand side of (3.7), using (2.35) and the mean-value theorem (MVT) we have

\[
\left| \hat{f}_i(\hat{u}^h) \right| \leq \left| \hat{f}_i(0) \right| + \left| \hat{f}_i(\hat{u}^h) - \hat{f}_i(0) \right|
\]

\[
\leq \left| \hat{f}_i(0) \right| + \bar{C} \sum_{j=1}^m |\hat{a}_j^3|,
\]

where \( \bar{C} \) is the Lipschitz constant of \( \hat{f} \). Therefore using (2.19) and (3.11) we have

\[
\left| \left\langle J \hat{f}_i(\hat{u}^h), \hat{u}_i^h \right\rangle_{\hat{\Omega}} \right| \leq \bar{C} \left( \sum_{j=1}^m \left| \hat{a}_j^3 \right|, \left| \hat{a}_i^3 \right| \right) + \left| \left\langle \hat{f}_i(0), \hat{u}_i^h \right\rangle_{\hat{\Omega}} \right|.
\]

Applying Young’s inequality gives

\[
\left| \left\langle J \hat{f}_i(\hat{u}^h), \hat{u}_i^h \right\rangle_{\hat{\Omega}} \right| \leq \bar{C} \left( \frac{1}{2} \sum_{j \neq i} \left| \hat{u}_j^h \right|_{L^2(\Omega_i)}^2 + \frac{m + 1}{2} \left| \hat{a}_i^3 \right|_{L^2(\Omega_i)}^2 \right)
\]

\[
+ \left| \hat{a}_i^3 \right|_{L^2(\Omega_i)}^2 + C_{\hat{f}_i(0)},
\]

where \( C_{\hat{f}_i(0)} \in \mathbb{R}^+ \) depends on \( |\hat{f}_i(0)| \). Summing over \( i \) we have

\[
\sum_{i=1}^m \left| \left\langle J \hat{f}_i(\hat{u}^h), \hat{u}_i^h \right\rangle_{\hat{\Omega}} \right| \leq \left( \bar{C} m + \frac{1}{2} \right) \left| \hat{u}^h \right|_{L^2(\Omega_r)}^2 + C_{\hat{f}(0)}.
\]

Using (2.22), (3.10) and (3.14) in (3.7) gives

\[
\frac{d}{dt} \left| \hat{u}^h \right|_{L^2(\Omega_r)}^2 + 2 \sum_{i=1}^m D_i \left| \nabla \hat{u}_i^h \right|_{L^2(\Omega_r)}^2 \leq \left( 2\bar{C} m + 1 - \nabla \cdot a \right) \left| \hat{u}^h, \hat{u}^h \right|_{\hat{\Omega}^m}^2 + 2C_{\hat{f}(0)}.
\]
Finally, integrating in time and applying Gronwall’s lemma we have

\begin{equation}
\left\| u^h(t) \right\|_{L^2(\Omega_t)^m}^2 \leq \left( \left\| u^h(0) \right\|_{L^2(\Omega_0)^m}^2 + 2tC_f(0) \right) \exp \left( \sup_\Omega \left\{ 2\tilde{C}m + 1 - \nabla \cdot \alpha \right\} t \right).
\end{equation}

From (2.17), the dilution term $\nabla \cdot \alpha$ has the same sign as $\partial_t J$ and is therefore positive (negative) if the domain is growing (contracting). Thus, domain growth has a diluting effect on the $L^2(\Omega_t)^m$ norm of the solution.

3.4. A priori analysis of the semidiscrete scheme. We now prove the error between the exact solution and the semidiscrete solution converges with optimal order in the $L^\infty(0, T; L^2(\hat{\Omega})^m)$ norm and the $L_2\left([0, T]; H^1(\hat{\Omega})^m\right)$ seminorm. A central role in the analysis is played by the Ritz (elliptic) projection originally introduced by Wheeler [34]. Given $\hat{\vartheta} \in H^1(\hat{\Omega})$, $\int_{\hat{\Omega}} \hat{\vartheta} = 0$, the Ritz projection $R^h : H^1(\hat{\Omega}) \to \hat{V}$ is defined to be the finite element solution of a corresponding elliptic problem:

\begin{equation}
\langle \nabla (\hat{\vartheta} - R^h \hat{\vartheta}), \nabla \tilde{\Phi} \rangle_{\hat{\Omega}} = 0 \quad \forall \tilde{\Phi} \in \hat{V},
\end{equation}

subject to the constraint

\begin{equation}
\int_{\hat{\Omega}} \hat{\vartheta} = \int_{\hat{\Omega}} R^h \hat{\vartheta}.
\end{equation}

The constraint (3.18) is needed to ensure the solvability of the elliptic problem and the corresponding (elliptic) finite element problem. With the Ritz projection as defined above we have the following expression for the time-derivative of (3.17):

\begin{equation}
\langle \nabla \partial_t (\tilde{\vartheta}_i - R^h \tilde{\vartheta}_i), \nabla \tilde{\Phi} \rangle_{\hat{\Omega}} = 0 \quad \forall \tilde{\Phi} \in \hat{V}.
\end{equation}

To obtain optimal error estimates, we now decompose the error into an elliptic error (the error between the Ritz projection and the exact solution) and a parabolic error (the error between the semidiscrete solution and the Ritz projection):

\begin{equation}
\tilde{u}^h - \tilde{u} = \left( u^h - R^h \tilde{u} \right) + \left( \tilde{R}^h - u \right) = \hat{\rho}^h + \tilde{\epsilon}^h.
\end{equation}

where the equality defines $\hat{\rho}^h = (\hat{\rho}_1^h, \ldots, \hat{\rho}_m^h)^T$ and $\hat{\epsilon} = (\hat{\epsilon}_1, \ldots, \hat{\epsilon}_m)^T$. The following Lemma follows from well known results for the approximation of the pure Neumann elliptic problem (see for example [6, Ch. 5, Th. 5.4.4]):

3.5. Lemma (Elliptic error). Suppose the exact solution $u$ to Problem (2.2) is in $H^{\ell+1}(\Omega_t)^m$ with $\partial_t u$ in $H^{\ell+1}(\Omega_t)^m$ where $\ell$ is the polynomial degree of the finite element space (3.2). Furthermore, suppose Assumption 2.6 (with $k = \ell$) holds. Finally, let $\tilde{u}$ be as defined in (2.19) and $R^h$ be the Ritz projection defined in (3.17). Then the following estimates hold for the error in the Ritz projection and its time-derivative:

\begin{equation}
\sup_{t \in [0, T]} \left\{ \left\| \tilde{R}^h \tilde{u}(t) - \tilde{u}(t) \right\|_{L^2(\hat{\Omega})^m}^2 + h^2 \sum_{i=1}^m \left\| \nabla \left( \tilde{R}^h \tilde{u}_i(t) - \tilde{u}_i(t) \right) \right\|_{L^2(\hat{\Omega})}^2 \right\} \leq C h^{2(\ell+1)},
\end{equation}
Applying Young’s inequality:

\[ (3.27) \]

Dealing with the first term on the right of (3.25) using (3.20) and the MVT we have

\[ C \]

where \( H \) is in \( \ell \) is independent of the mesh-size \( h \).

3.6. Theorem (A priori estimate for the semidiscrete scheme). Suppose the exact solution \( u \) to Problem (2.23) is in \( H^{\ell+1}(\Omega) \) with \( \partial_t u \) in \( H^{\ell+1}(\Omega) \), where \( \ell \) is the polynomial degree of the finite element space \( (3.2) \). Furthermore, suppose Assumption 2.6 (with \( k \) in place of \( \hat{k} \)) holds. Finally let \( \hat{u} \) be as defined in (2.19) and let \( \hat{u}^h \) be the solution to Problem (3.6). Then, the following optimal a priori error estimate holds for the error in the semidiscrete scheme:

\[ (3.28) \sup_{t \in [0, T]} \left\{ \left\| \partial_t \left( R^h \hat{u}(t) - \hat{u}(t) \right) \right\|_{L^2(\Omega)}^2 + \hat{h}^2 \sum_{i=1}^m \left\| \nabla \partial_t \left( R^h \hat{u}_i(t) - \hat{u}_i(t) \right) \right\|_{L^2(\Omega)}^2 \right\} \leq C \hat{h}^{2(\ell+1)}, \]

where \( C \in \mathbb{R}^+ \) is independent of the mesh-size \( h \).

Proof. Throughout the proof \( C \in \mathbb{R}^+ \) denotes an arbitrary constant independent of the mesh-size \( h \). Using decomposition (3.20) and Lemma 3.5 we have a bound on the elliptic error and it simply remains to estimate the parabolic error \( \rho^h \). To this end, we use (3.6) to construct a PDE for \( \hat{\rho}^h \) by inserting \( \rho^h \) in place of \( \hat{u}^h \) and taking \( \Phi = \rho^h \). Using (2.22) we obtain for \( i = 1, \ldots, m, \)

\[ (3.29) \left( \partial_t \left( J \rho^h \right), \rho^h \right) + D_1 \left\| \nabla \rho^h \right\|_{L^2(\Omega)}^2 = \left( \tilde{f}_i(\tilde{u}^h), J\rho^h \right) - \left( J K \nabla R^h \tilde{u}_i, K \nabla \rho^h \right). \]

Using (2.33), (2.36) and (3.17) gives

\[ (3.30) \left( \partial_t \left( J \rho^h \right), \rho^h \right) + D_1 \left\| \nabla \rho^h \right\|_{L^2(\Omega)}^2 = \left( \tilde{f}_i(\tilde{u}^h), J\rho^h \right) - \left( \partial_t \left( J \hat{\varepsilon} \right), \rho^h \right). \]

Dealing with the first term on the left of (3.30) as in (3.10):

\[ (3.31) \left( \partial_t \left( J \rho^h \right), \rho^h \right) = \frac{1}{2} \left( \frac{d}{dt} \left\| \rho^h \right\|_{L^2(\Omega)}^2 + \left( \rho^h \nabla : \hat{\alpha}, \rho^h \right) \right). \]

Dealing with the first term on the right of (3.30) using (3.20) and the MVT we have

\[ (3.32) \left| \left( \tilde{f}_i(\tilde{u}^h) - \tilde{f}_i(\tilde{u}), J\rho^h \right) \right| \leq \tilde{C} \left( \left( \sum_{j=1}^m \left| \hat{\varepsilon}_j \right| + \left| \hat{\rho}^h_j \right| \right) \left( \sum_{j=1}^m \left| \hat{\varepsilon}_j \right| \right) \right). \]

Applying Young’s inequality:

\[ (3.33) \left| \left( \tilde{f}_i(\tilde{u}^h) - \tilde{f}_i(\tilde{u}), J\rho^h \right) \right| \leq \tilde{C} \left( \left( m + \frac{1}{2} \left( \left\| \rho^h \right\|_{L^2(\Omega)}^2 + \sum_{j \neq i} \frac{1}{2} \left| \hat{\rho}^h_j \right| \right) \right) \right) + \frac{1}{2} \left( \left. \left| J \right|_{L^\infty([0,T])} \right| \left( \left. \left| \hat{\varepsilon} \right| \right| \right) \right) \left( \left. \left| \hat{\varepsilon} \right| \right| \right). \]
Summing over \(i\) we have
\[
\sum_{i=1}^{m} \left| \left\langle \tilde{f}_i (\tilde{u}^h) - \tilde{f}_i (\tilde{u}), J \hat{\rho}_i^h \right\rangle \right| \leq \tilde{C} \left( \frac{3m}{2} \left\| \rho^h \right\|_{L^2(\Omega_t)}^2 + \frac{m}{2} \left\| J \right\|_{L^\infty(\hat{\Omega} \times [0,T])} \left\| \tilde{\varepsilon} \right\|_{L^2(\hat{\Omega})}^2 \right).
\]
(3.29)

Dealing with the second term on the right of (3.25):
\[
\left| \left\langle \partial_t (J \hat{\varepsilon}_i), \hat{\rho}_i^h \right\rangle \right| \leq \left\| \left\langle J \partial_t \hat{\varepsilon}_i, \hat{\rho}_i^h \right\rangle \right\| + \left\| \left\langle \partial_t (J \hat{\varepsilon}_i), \hat{\rho}_i^h \right\rangle \right\|
\leq \frac{1}{2} \left( \left\| \rho^h \right\|_{L^2(\Omega_t)}^2 + \left\| J \partial_t \hat{\varepsilon}_i, \partial_t \hat{\varepsilon}_i \right\|_{\hat{\Omega}}^2 \right)
+ \left\| \left\langle \partial_t (J), \hat{\rho}_i^h \right\rangle \right\| + \left\| \left\langle \partial_t (J), \hat{\varepsilon}_i, \hat{\varepsilon}_i \right\rangle \right\|,
\]
(3.30)
where we have used Young’s inequality for the second step. Now using (2.17) and summing over \(i\) we have
\[
\sum_{i=1}^{m} \left| \left\langle \partial_t (J \hat{\varepsilon}_i), \hat{\rho}_i^h \right\rangle \right| \leq \frac{1}{2} \left( \left\| \rho^h \right\|_{L^2(\Omega_t)}^2 + \left\| \rho^h \right\|_{L^2(\Omega_t)} \left\| J \right\|_{L^\infty(\hat{\Omega} \times [0,T])} \left\| \hat{\varepsilon} \right\|_{L^2(\hat{\Omega})}^2 \right)
+ \left\| \partial_t J \right\|_{L^\infty(\hat{\Omega} \times [0,T])} \left\| \hat{\varepsilon} \right\|_{L^2(\hat{\Omega})}^2.
\]
(3.31)

Combining (3.26), (3.29), (3.31)
\[
\frac{d}{dt} \left\| \rho^h \right\|_{L^2(\Omega_t)}^2 + 2 \sum_{i=1}^{m} D_i \left\| \nabla \rho^h \right\|_{L^2(\Omega_t)}^2 \leq C \left( \left\| \rho^h \right\|_{L^2(\Omega_t)}^2 + \left\| \hat{\varepsilon} \right\|_{L^2(\hat{\Omega})}^2 \right)
+ \left\| \partial_t \hat{\varepsilon} \right\|_{L^2(\hat{\Omega})}^2,
\]
(3.32)
where we have used the fact that Assumption 2.6 implies \( J, \partial_t J \in L^\infty (\hat{\Omega} \times [0,T]) \). Integrating in time, using Lemma 3.5 and applying Gronwall’s Lemma we have
\[
\left\| \rho^h (t) \right\|_{L^2(\Omega_t)}^2 + 2 \sum_{i=1}^{m} D_i \int_0^T \left\| \nabla \rho^h \right\|_{L^2(\Omega_t)}^2 \leq C \left( \left\| \rho^h (0) \right\|_{L^2(\Omega_t)}^2 + \hat{h}^{2(\ell+1)} \right).
\]
(3.33)

To estimate \( \rho^h (0) \), we note
\[
\left\| \rho^h (0) \right\|_{L^2(\Omega_t)}^2 \leq C \left( \left\| \hat{u} (0) - \Lambda^h \hat{u} (0) \right\|_{L^2 (\hat{\Omega})}^2 + \left\| \tilde{\varepsilon}^h \right\|_{L^2 (\hat{\Omega})}^2 \right)
\leq C \hat{h}^{\ell+1},
\]
(3.34)
where we have used (3.3), the assumption on the regularity of the exact solution and Lemma 3.5 in the last step. Assumption 2.6 and the equivalence of norms on the reference and evolving domains (2.21) completes the proof.
3.7. Fully discrete approximation. We now propose a time discretisation of (3.6). To this end, we divide the time interval \([0, T]\) into \(N\) equal-length subintervals, \(0 = t_0 < \ldots < t_N = T\) and denote by \(\tau := t_n - t_{n-1}\) the time step. We consistently use the following shorthand for a function of time: \(f^n := f(t_n)\), we denote by \(\hat{f}^n := \tau^{-1} \left( f^n - f^{n-1} \right)\).

For the approximation in time we use a finite difference scheme, specifically the 1-SBEM a modified implicit Euler method where linear reaction terms and the diffusive term are treated implicitly while the nonlinear reaction terms are treated semi-implicitly using values from the previous timestep (a 1-step Picard linearisation). Our choice of timestepping scheme stems from the numerical investigation conducted by Madzvamuse [20], where the 1-SBEM was deemed to be robust for the applications we have in mind.

The fully discrete scheme we employ to approximate the solution of Problem (2.23) is thus, find \(\bar{U}_n^m \in \bar{\mathcal{V}}\), for \(n = 1, \ldots, N\), such that for \(i = 1, \ldots, m\), we have

\[
\begin{aligned}
\left\{ \begin{array}{l}
\frac{\partial}{\partial t} \left[ U_i^n \right] + D_i \left[ \nabla U_i^n , \nabla \Phi^n \right]_{\Omega_n} = \left( J^n f_i \left( \bar{U}_n^m , \bar{U}^{n-1} \right) , \Phi \right)_\Omega , \quad \forall \Phi \in \mathcal{V}, \\
\bar{U}_0^i = \Lambda^h u_0^i,
\end{array} \right.
\end{aligned}
\tag{3.35}
\]

where \(\Lambda^h\) is the Lagrange interpolant.

Alternatively we may look to approximate the solution to (2.23) on a conforming subspace of the evolving domain. To this end we define a family of finite dimensional spaces \(\mathcal{V}^n, n = [0, \ldots, N]\) such that with \(\Phi\) as defined in (3.2):

\[
\forall^n := \left\{ \Phi^n \in H^1(\Omega_n) : \Phi^n(\mathcal{A}(\xi, t_n)) = \hat{\Phi}(\xi) \right\},
\tag{3.36}
\]

which also defines the triangulation \(\mathcal{T}^n, n = [0, \ldots, N]\) on the evolving domain. Using (3.35) and (3.36) we have the following equivalent finite element formulation on the evolving domain: find \(U_i^n \in \forall^n\), for \(n = 1, \ldots, N\), such that for \(i = 1, \ldots, m\),

\[
\begin{aligned}
\left\{ \begin{array}{l}
\frac{\partial}{\partial t} \left[ U_i^n \right] + D_i \left[ \nabla U_i^n , \nabla \Phi^n \right]_{\Omega_n} = \left( J^n f_i \left( U_i^n , U^{n-1} \right) , \Phi^n \right)_\Omega , \\
U_i^0 = \Lambda^h u_0^i,
\end{array} \right.
\end{aligned}
\tag{3.37}
\]

where \(\Lambda^h : H^1(\Omega_0) \rightarrow \mathcal{V}_0\) is the Lagrange interpolant. By (2.20) and (3.36)

\[
\begin{aligned}
\partial_t \hat{\Phi}(\xi) = [\partial_t \hat{\Phi} + a \cdot \nabla \hat{\Phi}] (\mathcal{A}(\xi, t)) = 0.
\end{aligned}
\tag{3.38}
\]

Thus, (3.37) may be viewed as a finite element discretisation of the formulation (2.34).

3.8. Theorem (A priori estimate for the fully discrete scheme). Suppose the exact solution \(u\) to Problem (2.23) is in \(H^{t+1}(\Omega)^m\) with \(\partial_t u \in H^{t+1}(\Omega)^m\) where \(t\) is the polynomial degree of the finite element space (3.2). Furthermore, suppose Assumption 2.6 (with \(k = \ell\)) holds. Let \(\hat{u}\) be as defined in (2.19) and let \(\bar{U}\) be the solution to (3.35). Finally, suppose the timestep satisfies a stability condition defined in (3.49). Then, the following optimal a priori estimate holds for the error in the fully discrete scheme:

\[
\| \bar{U}^n - \hat{u}^n \|_{L_2(\Omega)}^2 \leq C \left( \hat{h}^{2(t+1)} + \tau^2 \right) \quad \text{for } n \in [0, \ldots, N],
\tag{3.39}
\]

where \(C \in \mathbb{R}^+\) is independent of the mesh-size \(\hat{h}\) and the timestep \(\tau\).
Proof. Throughout the proof $C \in \mathbb{R}^+$ denotes an arbitrary constant independent of the mesh-size $\hat{h}$ and the timestep $\tau$. Decomposing the error as in (3.20) we have

\[
\| \bar{U}_h^n - \hat{u}_h^n \|_{L^2(\hat{\Omega})}^m \leq \| R^h \bar{U}_h^n - \hat{u}_h^n \|_{L^2(\hat{\Omega})}^m + \| \bar{U}_h^n - R^h \hat{u}_h^n \|_{L^2(\hat{\Omega})}^m 
\]

(3.40)

From Lemma 3.3 we have the following bound on the elliptic error:

\[
\| \hat{e}_h^n \|_{L^2(\hat{\Omega})}^m \leq C \hat{h}^{2(\ell + 1)} \quad \text{for } n \in \{0, \ldots, N\}.
\]

(3.41)

Therefore it only remains to estimate $\hat{\rho}_h^n$. Constructing an expression for $\hat{\rho}_h^n$ as in (3.24), using (3.35) and (3.17) we obtain for $i = 1, \ldots, m,$

\[
\langle \partial_i [J \hat{\rho}_h^n], \hat{\rho}_h^n \rangle_{\hat{\Omega}} + D_i \| \nabla \hat{\rho}_h^n \|_{L^2(\hat{\Omega})}^2 = \left\langle \bar{f}_i(\bar{U}_h^n, \bar{U}_h^{n-1}), \langle J \hat{\rho}_h^n \rangle \right\rangle_{\hat{\Omega}}
\]

- \langle \partial_i [J R^h \hat{u}_h^n], \hat{\rho}_h^n \rangle_{\hat{\Omega}} - D_i \langle [J K \nabla \hat{u}_h^n], \langle K \nabla \hat{\rho}_h^n \rangle \rangle_{\hat{\Omega}}

(3.42)

where we have used (2.33) for the second step. Using Young’s inequality for the first term on the left hand side of (3.42) gives

\[
\langle \partial_i [J \hat{\rho}_h^n], \hat{\rho}_h^n \rangle_{\hat{\Omega}} \geq \frac{1}{\tau} \| \hat{\rho}_h^n \|_{L^2(\hat{\Omega})}^2 - \frac{1}{2} \left( \langle J^{n-1} \hat{\rho}_h^n, \hat{\rho}_h^n \rangle_{\hat{\Omega}} + \langle J^n \hat{\rho}_h^n, \hat{\rho}_h^n \rangle_{\hat{\Omega}} \right).
\]

(3.43)

where we have used (2.21). Summing over $i$ we have

\[
\sum_{i=1}^{m} \langle \partial_i [J \hat{\rho}_h^n], \hat{\rho}_h^n \rangle_{\hat{\Omega}} \geq \frac{1}{\tau} \left( 1 - \frac{1}{2} \left\| J^{n-1} \right\|_{L^\infty(\hat{\Omega})} \left\| \hat{\rho}_h^n \right\|_{L^2(\hat{\Omega})}^m \right) - \frac{1}{2\tau} \| \hat{\rho}_h^{n-1} \|_{L^2(\hat{\Omega})}^m.
\]

(3.44)

Using (3.40) and the MVT for the first term on the right of (3.42) gives

\[
\left| \left\langle \bar{f}_i(\bar{U}_h^n, \bar{U}_h^{n-1}) - \bar{f}_i(\hat{u}_h^n), \langle J \hat{\rho}_h^n \rangle \right\rangle_{\hat{\Omega}} \right|
\]

\[
\leq \tilde{C} \sum_{j=1}^{m} \left( \| \hat{e}_j^{n-1} \|_{L^\infty(\hat{\Omega})} + \| J \hat{\rho}_h^n \|_{L^\infty(\hat{\Omega})} \right) \left( \| \hat{\rho}_h^{n-1} \|_{L^2(\hat{\Omega})} + \| J^n \|_{L^\infty(\hat{\Omega})} \right) \| \hat{e}_j^{n-1} \|_{L^2(\hat{\Omega})}^m + \| J^n \|_{L^\infty(\hat{\Omega})} \left( \| \hat{e}_j^n \|_{L^2(\hat{\Omega})}^m + \| \hat{e}_j^{n-1} \|_{L^2(\hat{\Omega})}^m \right).
\]

(3.45)
where we have used Young’s inequality for the second step. Summing over $i$ we have

$$
\sum_{i=1}^{m} \left| \langle \tilde{f}_i(U_i^n, \tilde{U}^{n-1}) - \tilde{f}_i(\tilde{u}^n), [J \rho]^n \rangle \right| \leq C \tilde{C} \left( \|\rho^n\|_{L^2(\Omega_n)^m}^2 + \left\| J^n \right\|_{L^\infty(\hat{\Omega})} \left\| \rho^{n-1} \right\|_{L^2(\Omega_{n-1})}^2 \\
+ \|J^n\|_{L^\infty(\hat{\Omega})} \left( \|\tilde{\varepsilon}^n\|_{L^2(\hat{\Omega})}^2 + \|\tilde{\varepsilon}^{n-1}\|_{L^2(\hat{\Omega})}^2 \right) \right).
$$

Applying Young’s inequality to the second and third term on the right of (3.42) gives

$$
\left| \langle \tilde{\varepsilon}_i^n, \rho_i^n \rangle \right| + \left| \langle (\tilde{\varepsilon} - \partial_t) [J \tilde{u}_i]^n, \rho_i^n \rangle \right| \\
\leq \|\rho_i^n\|_{L^2(\Omega_n)}^2 + \frac{1}{2} \left\| J^n \right\|_{L^\infty(\hat{\Omega})} \left( \|\tilde{\varepsilon}_i^n\|_{L^2(\hat{\Omega})}^2 + \left\| (\tilde{\varepsilon} - \partial_t) [J \tilde{u}_i]^n \right\|_{L^2(\hat{\Omega})}^2 \right).
$$

Using (3.44), (3.46) and (3.47) in (3.42) gives

$$
\frac{1}{\tau} \left( 1 - \frac{1}{2} \left\| J^n \right\|_{L^\infty(\hat{\Omega})} - C \tilde{C} \right) \left( \|\rho^n\|_{L^2(\Omega_n)^m}^2 + \sum_{i=1}^{m} D_i \|\nabla \rho_i^n\|_{L^2(\Omega_i)}^2 \right) \\
\leq \left( \frac{1}{2\tau} + C \tilde{C} \right) \left\| J^n \right\|_{L^\infty(\hat{\Omega})} \left( \|\tilde{\varepsilon}^n\|_{L^2(\hat{\Omega})}^2 + \|\tilde{\varepsilon}^{n-1}\|_{L^2(\hat{\Omega})}^2 \right) \\
+ C \tilde{C} \left\| J^n \right\|_{L^\infty(\hat{\Omega})} \left( \|\tilde{\varepsilon}_i^n\|_{L^2(\hat{\Omega})}^2 + \left\| (\tilde{\varepsilon} - \partial_t) [J \tilde{u}_i]^n \right\|_{L^2(\hat{\Omega})}^2 \right).
$$

Let $\tau' > 0$ be such that, for $\tau < \tau'$

$$
1 - \frac{1}{2} \left\| J^n \right\|_{L^\infty(\hat{\Omega})} - C \tilde{C} \tau > 0.
$$

Such a $\tau'$ exists since

$$
\lim_{\tau \to 0} \left\{ \frac{1}{2} \left\| J^n \right\|_{L^\infty(\hat{\Omega})} + C \tilde{C} \right\} = \frac{1}{2}.
$$

For $\tau < \tau'$, we have

$$
\|\rho^n\|_{L^2(\Omega_n)^m}^2 + \sum_{i=1}^{m} C \tau D_i \|\nabla \rho_i^n\|_{L^2(\Omega_i)}^2 \leq C \left( \tilde{C} \left\| \rho^{n-1} \right\|_{L^2(\Omega_{n-1})}^2 + \tau R^n \right).
$$
where \( C^n = 1 + \tau \tilde{C} \left\| \frac{J^n}{J^n} \right\|_{L_\infty (\hat{\Omega})} \) and

\[
\mathcal{R}^n := \tilde{C} \left\| J^n \right\|_{L_\infty (\hat{\Omega})} \left( \left\| \tilde{\varepsilon}^n \right\|^2_{L^2 (\hat{\Omega})} + \left\| \tilde{\varepsilon}^{n-1} \right\|^2_{L^2 (\hat{\Omega})} + \left\| \tau \tilde{\partial} \tilde{u}^n \right\|^2_{L^2 (\hat{\Omega})} \right) \\
+ \frac{\tau}{2} \left\| \frac{1}{J^n} \right\|_{L_\infty (\hat{\Omega})} \left( \left\| [\hat{J} \tilde{\varepsilon}]^n \right\|^2_{L^2 (\hat{\Omega})} + \left\| (\tilde{\pi} - \partial_t) [J \tilde{u}]^n \right\|^2_{L^2 (\hat{\Omega})} \right).
\]

(3.52)

Therefore, for \( n \in [1, \ldots, N] \),

\[
\left\| \rho^n \right\|^2_{L^2 (\Omega^n)} + \sum_{i=1}^{m} C \tau D_i \left\| \nabla \rho^n \right\|^2_{L_\infty (\Omega_i)} \leq C \left( \prod_{k=1}^{n} \tilde{C}^k \left\| \rho^0 \right\|^2_{L_2 (\Omega_0)} \right) + \tau \prod_{j=1}^{n} \tilde{C}^j \mathcal{R}^j.
\]

(3.53)

Considering the first two terms on the right of (3.52), we have for \( n \in [1, \ldots, N] \)

\[
\tilde{C} \left\| J^n \right\|_{L_\infty (\hat{\Omega})} \left( \left\| \tilde{\varepsilon}^n \right\|^2_{L^2 (\hat{\Omega})} + \left\| \tilde{\varepsilon}^{n-1} \right\|^2_{L^2 (\hat{\Omega})} \right) \leq 2 \tilde{C} \sup_{s \in [0, \ldots, N]} \left\| J^s \right\|_{L_\infty (\hat{\Omega})} \left\| \tilde{\varepsilon}^s \right\|^2_{L^2 (\hat{\Omega})} \leq \tilde{C} C \hat{h}^{2(\tau + 1)},
\]

where we have used Assumption 2.6 and Lemma 3.5. Dealing with the third term on the right of (3.52), we have

\[
\tilde{C} \left\| J^n \right\|_{L_\infty (\hat{\Omega})} \left\| \tau \tilde{\partial} \tilde{u}^n \right\|^2_{L^2 (\hat{\Omega})} = \tilde{C} \left\| J^n \right\|_{L_\infty (\hat{\Omega})} \left\| \int_{t^{n-1}}^{t^n} \partial_t \tilde{s} ds \right\|^2_{L^2 (\hat{\Omega})} \leq \tilde{C} C \tau^2,
\]

(3.55)

where we have used Assumptions 2.4, 2.6, and 2.28. For the fourth term on the right of (3.52) we have

\[
\frac{1}{2} \left\| \frac{1}{J^n} \right\|_{L_\infty (\hat{\Omega})} \left\| [\hat{J} \tilde{\varepsilon}]^n \right\|^2_{L^2 (\hat{\Omega})} \leq \frac{1}{2} \left\| \frac{1}{J^n} \right\|_{L_\infty (\hat{\Omega})} \left\| \frac{1}{\tau} \int_{t^{n-1}}^{t^n} \partial_t [J \tilde{u}]^n ds \right\|^2_{L^2 (\hat{\Omega})} \leq C \sup_{s \in [t^{n-1}, t^n]} \left\| [\tilde{s}]^n \right\|^2_{L^2 (\hat{\Omega})} \leq C \hat{h}^{2(\tau + 1)},
\]

(3.56)

where we have used Assumption 2.6 for the second step and Lemma 3.5 for the final step. Finally, for the fifth term on the right of (3.52) we have

\[
\left\| \frac{1}{J^n} \right\|_{L_\infty (\hat{\Omega})} \left\| (\tilde{\pi} - \partial_t) [J \tilde{u}]^n \right\|^2_{L^2 (\hat{\Omega})} \leq \left\| \frac{1}{J^n} \right\|_{L_\infty (\hat{\Omega})} \left\| \frac{1}{\tau} \int_{t^{n-1}}^{t^n} (s - t^{n-1}) \partial_t [J \tilde{u}]^n ds \right\|^2_{L^2 (\hat{\Omega})} \leq C \tau^2 \sup_{s \in [t^{n-1}, t^n]} \left( \left\| \partial_t \tilde{u}^s \right\|^2_{L^2 (\hat{\Omega})} + \left\| \tilde{u}^s \right\|^2_{L^2 (\hat{\Omega})} \right) \leq C \tau^2,
\]

(3.57)
where we have used Assumption 2.6 for the second step and Assumption 2.4 for the final step. Combining (3.54), (3.55), (3.56) and (3.57) we have

\[ R^n \leq C \left( \hat{h}^{2(\ell+1)} + \tau^2 \right) \text{ for } n \in [1, \ldots, N]. \]  

Using (3.5) gives

\[ (3.62) \]

\[ \hat{\rho}_n(h^2) \leq C \hat{h}^{2(\ell+1)}. \]

Remark 3.9. Applying estimates (3.58) and (3.59) in (3.51) completes the proof of Theorem 3.8. \( \Box \)

3.9. Remark (Stability of the fully discrete scheme). The timestep restriction (3.49) is composed of a term arising from domain growth (the term involving the determinant \( J \)) and a term arising from the nonlinear reaction kinetics (the term containing \( \hat{C} \)). It is worth noting that for a given set of reaction kinetics, i.e., a given \( \hat{C} \), larger timesteps are admissible on growing domains (as the term \( \frac{\max h^2}{\tau} \leq L_\infty(\hat{\Omega}) \) is not explicitly known. Thus, we cannot construct the function \( \hat{f} \) defined in (2.35). To this end, we introduce the following assumption to circumvent the construction of \( \hat{f} \).

3.10. Assumption (Dimension dependent polynomial degree). We wish to invoke estimate (3.4) with a positive power of \( \hat{h} \) and thus we require the degree of the finite element space to satisfy

\[ \ell > \frac{d}{2} - 1, \]

where \( d \) is the spatial dimension. Thus, we require piecewise linear or higher basis functions for \( d \leq 2 \) and at least piecewise quadratics for \( d = 3 \).

3.11. Assumption (Assumption 3.11). For sufficiently small mesh-size \( \hat{h} \) the discrete solution \( \hat{U}^n \) to Problem (3.35) is in the region \( I_\delta \) for all \( n \in [0, \ldots, N] \). Thus, we may replace \( \hat{f} \) in (3.35) by \( f \).

Proof. For \( n \in [0, \ldots, N] \) we have for \( T^h \) the Clément interpolant

\[ \| \hat{u}^n - \hat{U}^n \|_{L_{\infty}(\hat{\Omega})} \leq \| T^h \hat{u}^n - \hat{U}^n \|_{L_{\infty}(\hat{\Omega})} + \| \hat{u}^n - T^h \hat{u}^n \|_{L_{\infty}(\hat{\Omega})}. \]  

By (3.4) we have

\[ \| \hat{u}^n - \hat{U}^n \|_{L_{\infty}(\hat{\Omega})} \leq C \left( \hat{h}^{\ell+1-d/2} \| \hat{u}^n \|_{H^{\ell+1}(\hat{\Omega})} \right). \]

(3.62)

Using (3.5) gives

\[ \| \hat{u}^n - \hat{U}^n \|_{L_{\infty}(\hat{\Omega})} \leq C \left( \hat{h}^{\ell+1-d/2} \| \hat{u}^n \|_{H^{\ell+1}(\hat{\Omega})} \right). \]

(3.63)
For reaction kinetics (4.1) the components of \( \hat{\mathbf{u}} \) and (4.4) respectively. The components of \( \hat{\mathbf{u}} \) where \( W \) is taken sufficiently small we have

\[
\sup_{n \in [0, \ldots, N]} \| \hat{\mathbf{u}}^n - \hat{\mathbf{U}}^n \|_{L^\infty (\hat{\Omega})} \leq \delta/2,
\]

Therefore, \( \hat{\mathbf{U}}^n \in I_\delta \) for all \( n \in [0, \ldots, N] \) and thus, \( \tilde{f}(\hat{\mathbf{U}}) = f(\hat{\mathbf{U}}) \) completing the proof.

4. IMPLEMENTATION

In this section we illustrate the implementation of the finite element scheme with explicit nonlinear reaction functions. We demonstrate that scheme (3.35) on the reference domain or scheme (3.37) on the evolving domain give rise to equivalent linear systems. To illustrate a concrete application of the proposed scheme we consider the following widely studied set of reaction kinetics.

4.1. Definition (Schnakenberg (Activator-depleted substrate) model). \([12, 16, 26]\) We consider the activator-depleted substrate model also known as the Brusselator model:

\[
\begin{cases}
    f_1 (u_1, u_2) = \gamma (a - u_1 + u_1^2 u_2), \\
    f_2 (u_1, u_2) = \gamma (b - u_1^2 u_2),
\end{cases}
\]

where \( 0 < a, b, \gamma < \infty \).

In matrix vector form scheme (3.35) equipped with kinetics (4.1) and appropriate initial approximations \( W_1^0, W_2^0 \) is: To solve for \( W_1^n, W_2^n \), \( n = [1, \ldots, N] \), the linear systems given by

\[
\begin{align*}
    \left( \frac{1}{2} \hat{\mathbf{M}}^n + D_1 \hat{\mathbf{S}}^n + \gamma \hat{\mathbf{N}}_1^n \right) \hat{\mathbf{W}}_1^n &= \frac{1}{2} M^{n-1} \hat{\mathbf{W}}_1^{n-1} + \gamma a \hat{\mathbf{F}}^n, \\
    \left( \frac{1}{2} \hat{\mathbf{M}}^n + D_2 \hat{\mathbf{S}}^n + \gamma \hat{\mathbf{N}}_2^n \right) \hat{\mathbf{W}}_2^n &= \frac{1}{2} M^{n-1} \hat{\mathbf{W}}_2^{n-1} + \gamma b \hat{\mathbf{F}}^n,
\end{align*}
\]

where \( \hat{\mathbf{W}}_1 \) and \( \hat{\mathbf{W}}_2 \) represent the nodal values of the discrete solutions corresponding to \( \hat{u}_1 \) and \( \hat{u}_2 \) respectively. The components of \( \hat{\mathbf{M}}, \hat{\mathbf{S}} \) and \( \hat{\mathbf{F}} \) are given by

\[
\begin{align*}
    \hat{\mathbf{M}}_{\alpha\beta} &= \int_{\Omega} J^n \hat{\Phi}_\alpha \hat{\Phi}_\beta, \\
    \hat{\mathbf{S}}_{\alpha\beta} &= \int_{\Omega} [J K^n] \nabla \hat{\Phi}_\alpha \cdot K^n \nabla \hat{\Phi}_\beta, \\
    \hat{\mathbf{F}}_{\alpha} &= \int_{\Omega} J^n \hat{\Phi}_\alpha.
\end{align*}
\]

For reaction kinetics (4.1) the components of \( \hat{\mathbf{N}}_1 \) and \( \hat{\mathbf{N}}_2 \) are given by

\[
\begin{align*}
    \left( \hat{\mathbf{N}}_1 \right)_{\alpha\beta} &= \sum_{\eta=1}^{\dim(\mathcal{V})} \sum_{\vartheta=1}^{\dim(\mathcal{V})} [(W_1)_\eta(W_2)_\vartheta]^{n-1} \int_{\Omega} J^n \hat{\Phi}_\eta \hat{\Phi}_\beta \hat{\Phi}_\vartheta, \\
    \left( \hat{\mathbf{N}}_2 \right)_{\alpha\beta} &= \int_{\Omega} J^n \hat{\Phi}_\alpha \hat{\Phi}_\beta + \sum_{\eta=1}^{\dim(\mathcal{V})} \sum_{\vartheta=1}^{\dim(\mathcal{V})} [(W_1)_\eta(W_2)_\vartheta]^{n-1} \int_{\Omega} J^n \hat{\Phi}_\eta \hat{\Phi}_\beta \hat{\Phi}_\vartheta,
\end{align*}
\]

respectively.
We now illustrate the implementation of scheme \(3.37\) where the linear systems are assembled on the evolving domain. By the definition of \(\mathcal{V}_n\) \((3.36)\) we obtain the following system matrices if we assemble the linear systems on the evolving domain

\[
M^n_{\alpha\beta} := \int_{\Omega_n} \Phi_n^\alpha \Phi_n^\beta = \hat{M}_n^{\alpha\beta},
\]
\[
S^n_{\alpha\beta} := \int_{\Omega_n} \nabla \Phi_n^\alpha \cdot \nabla \Phi_n^\beta = \hat{S}_n^{\alpha\beta},
\]
and
\[
F_n^\alpha := \int_{\Omega_n} \Phi_n^\alpha = \hat{F}_n^{\alpha}.
\]

We thus obtain the following linear systems:

\[
\begin{aligned}
\left\{ 
\frac{1}{2} M^n + D_1 S^n + \gamma N_1^n \right\} W_1^n &= \frac{1}{2} M^{n-1} W_1^{n-1} + \gamma a F^n \\
\left\{ \frac{1}{2} M^n + D_2 S^n + \gamma N_2^n \right\} W_2^n &= \frac{1}{2} M^{n-1} W_2^{n-1} + \gamma b F^n,
\end{aligned}
\]

where for reaction kinetics \((4.1)\) the components of \(N_1 = \hat{N}_1\) are given by

\[
(N_1)^{\alpha\beta} := \sum_{\eta=1}^{\dim(\mathcal{V})} \sum_{\vartheta=1}^{\dim(\mathcal{V})} [(W_2)_\eta (W_2)_\vartheta]^{n-1} \int_{\Omega_n} \Phi_n^\alpha \Phi_n^\beta \Phi_n^\eta \Phi_n^\vartheta
\]

with analogous modifications for \(N_2\).

Both formulations \((4.2)\) and \((3.37)\) result in the same linear algebra problem. Solve for vectors \(b_n^i, i = 1, \ldots, m,\)

\[
A^n b_n^i = c_i^{n-1}, \text{ for } n = 1, \ldots, N.
\]

The matrix \(A^n\) is symmetric sparse and positive definite. We therefore use the conjugate gradient (CG) algorithm [13] to compute the solution to the linear systems.

\[x = A(\xi, t)\]

\[\hat{h}_i\]

**Figure 1.** An example of the reference and evolving domain with the associated mapping, mesh-size and triangulations.
4.2. Remark (Quadrature on the evolving domain). As we do not have to compute the Jacobian of the mapping, assemblage of the linear systems is faster on the evolving domain. However, in the previous analysis we have neglected errors due to variational crimes, such as the fact that integrals of finite element functions must be evaluated by some numerical quadrature. Furthermore, simplices on the evolving domain will not in general be affine transformations of the reference simplex (see Figure 1 for an example). If formulation (3.37) is used and domain evolution is not spatially linear, the influence of numerical quadrature on the accuracy of the scheme should be considered. We leave this extension for future studies.

5. Numerical experiments

We now provide numerical evidence to back-up the estimate of Theorem 3.8. We use as a test problem, the Schnakenberg kinetics, although any other reaction kinetics that fulfill our assumptions could have been used.

5.1. Remark (Existence of solutions to Problem (2.23) with spatially linear isotropic evolution). In [32], we show that Problem (2.23) equipped with the Schnakenberg reaction kinetics and $\Omega_t \in C^2(\Omega_t)$ is well posed under any bounded spatially linear isotropic evolution of the domain. If we assume this result holds on polygonal domains, we have sufficient regularity on the continuous problem to apply Theorem 3.8 and thus conclude scheme (3.35) with $P_1$ finite elements converges with optimal order.

5.2. Definition (Experimental order of convergence). We denote the $L_\infty(0, T; L^2(\Omega))$ error in the numerical scheme on a series of uniform refinements of a triangulation $\{\mathcal{T}_i\}_{i=0,...,N}$ by $\{e_i\}_{i=0,...,N}$. The experimental order of convergence (EOC) is defined to be the numerical measure of rate of convergence of the scheme as $\hat{h}_n \to 0$, where $\hat{h}_n$ denotes the maximum mesh-size of $\mathcal{T}_n$ and is given by

$$\text{EOC}_i(e_{i,i+1}, \hat{h}_{i,i+1}) = \frac{\ln(e_{i+1}/e_i)}{\ln(\hat{h}_{i+1}/\hat{h}_i)}.$$  

5.3. Numerical verification of the a priori convergence rate. We examine the EOC of scheme (3.35) to approximate the solution to (2.23) with $P_1$, $P_2$ and $P_3$ basis functions and with timestep $\tau \approx \hat{h}^2$, $\tau \approx \hat{h}^3$ and $\tau \approx \hat{h}^4$ respectively (since the scheme is first order in time).

We consider two different forms of domain evolution that include both domain growth and contraction to illustrate the versatility of the proposed finite element scheme.

- Spatially linear periodic evolution:

$$A_0(\xi, t) = \xi \left( 1 + \kappa \sin \left( \frac{\pi t}{T} \right) \right).$$

- Spatially nonlinear periodic evolution:

$$A_i(\xi_i, t) = \xi_i \left( 1 + \kappa \sin \left( \frac{\pi t}{T} \right) \xi_i \right),$$

for $i = 1, \ldots, d$.

In both cases we take a time interval of $[0, 1]$, the initial domain as the unit square and the parameter $\kappa = 1$. Thus in both cases the domain grows to a square of length 2 at $t = 0.5$ before contracting back to the initial domain at end time. We take the diffusion coefficients $D = (0.01, 1)^T$ and the parameter $\gamma = 1$. Problem (2.23) equipped with nonlinear reaction kinetics does not admit any closed form solutions. In
order to provide numerical verification of the convergence rate, we insert a source term such that the exact solution is,

\[
\hat{u}_1(\xi, t) = \sin(\pi t) \exp(-10 |\xi|^2),
\]

\[
\hat{u}_2(\xi, t) = -\sin(\pi t) \exp(-10 |\xi|^2).
\]

(5.4)

Tables 1 and 2 show the EOCs for the two benchmark examples. For the first benchmark example where domain growth is linear with respect to space, we assemble the linear systems on the evolving domain corresponding to scheme (4.11). For the second benchmark example, as domain evolution is nonlinear, we assemble the linear systems on the reference frame corresponding to scheme (4.2). In both cases we observe that the error converges at the expected rate of \( \ell + 1 \) where \( \ell \) is the degree of the finite element basis functions, providing numerical evidence for the a priori estimate of Theorem 3.8.

<table>
<thead>
<tr>
<th>( \hat{h} )</th>
<th>2(^{-5/2})</th>
<th>2(^{-3})</th>
<th>2(^{-7/2})</th>
<th>2(^{-4})</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p^1 )</td>
<td>( e )</td>
<td>0.119869</td>
<td>0.079248</td>
<td>0.040833</td>
</tr>
<tr>
<td>EOC</td>
<td>-</td>
<td>1.1940</td>
<td>1.9132</td>
<td>1.9853</td>
</tr>
<tr>
<td>( p^2 )</td>
<td>( e )</td>
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<td>0.012380</td>
<td>0.004405</td>
</tr>
<tr>
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<td>-</td>
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<td>2.981594</td>
<td>2.98227</td>
</tr>
<tr>
<td>( \hat{h} )</td>
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<td>2(^{-2})</td>
<td>2(^{-5/2})</td>
<td>2(^{-3})</td>
</tr>
<tr>
<td>( p^3 )</td>
<td>( e )</td>
<td>0.153871</td>
<td>0.042748</td>
<td>0.010899</td>
</tr>
<tr>
<td>EOC</td>
<td>-</td>
<td>3.6956</td>
<td>3.9433</td>
<td>3.9966</td>
</tr>
</tbody>
</table>

**TABLE 1.** Error in the \( L_\infty(0, T; L_2(\hat{\Omega})^m) \) norm and EOCs for a benchmark problem with spatially linear domain evolution (5.2). The linear systems are assembled on the evolving frame corresponding to system (4.11).

<table>
<thead>
<tr>
<th>( \hat{h} )</th>
<th>2(^{-5/2})</th>
<th>2(^{-3})</th>
<th>2(^{-7/2})</th>
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<tr>
<td>( p^1 )</td>
<td>( e )</td>
<td>0.043839</td>
<td>0.022429</td>
<td>0.011133</td>
</tr>
<tr>
<td>EOC</td>
<td>-</td>
<td>1.9337</td>
<td>2.0210</td>
<td>2.0441</td>
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<tr>
<td>( p^2 )</td>
<td>( e )</td>
<td>0.015906</td>
<td>0.005659</td>
<td>0.002005</td>
</tr>
<tr>
<td>EOC</td>
<td>-</td>
<td>2.9822</td>
<td>2.9941</td>
<td>3.0010</td>
</tr>
<tr>
<td>( \hat{h} )</td>
<td>2(^{-3/2})</td>
<td>2(^{-2})</td>
<td>2(^{-5/2})</td>
<td>2(^{-3})</td>
</tr>
<tr>
<td>( p^3 )</td>
<td>( e )</td>
<td>0.022086</td>
<td>0.005514</td>
<td>0.001375</td>
</tr>
<tr>
<td>EOC</td>
<td>-</td>
<td>4.0038</td>
<td>4.0068</td>
<td>4.0007</td>
</tr>
</tbody>
</table>

**TABLE 2.** Error in the \( L_\infty(0, T; L_2(\hat{\Omega})^m) \) norm and EOCs for a benchmark problem with nonlinear domain evolution (5.3). The linear systems are assembled on the reference frame corresponding to system (4.2).
5.4. **Spatial pattern formation on growing domains.** We now present numerical results illustrating the influence of domain evolution on pattern formation by RDSs. We first present results for the Schnakenberg kinetics with domain growth functions (5.2) and (5.3) with identical initial conditions and identical numerical and reaction kinetic parameter values as given in Table 3.

We take the unit square as the initial domain and the evolution of the boundary curve of the domain is identical in both cases, with the domain growing from a square of length 1 to a square of length 5 at \( t = 1000 \) before contracting to a square of length 1 at final time. In Figures 2 and 3 we show snapshots of the discrete activator \((W_1)\) profiles obtained using the different schemes. The substrate profiles \((W_2)\) have been omitted as they are \(180^\circ\) out of phase with those of the activator. The snapshots in Figure 2 were computed using the evolving domain formulation (4.11), whilst the snapshots in Figure 3 were computed using the reference domain formulation (4.2). Considering the Figures 2 and 3 we observe that no patterns are expressed when the domain is at initial or final times. This is as expected since linear stability analysis on a fixed square with the same length as the domain at \( t = 0 \), indicates that, for the set of parameter values selected, the domain is below the critical domain size for which there exist admissible patterns. In the spatially linear case (Figure 2), an initial half spot pattern forms which continuously transitions as the domain grows into a single spot positioned in the center of the domain. As the domain contracts this single spot disappears (via spot annihilation) with the final domain exhibiting no spatial patterning. In the spatially nonlinear growth case (Figure 3) the pattern transition is completely different with a half spot forming which splits as the domain grows to form two half spots which move around the domain before being annihilated as the domain contracts. The difference in patterning observed appears to be due to the differences in the growth function, with the results clearly illustrating the robustness of the numerical method in dealing with the complex non-uniform forms of domain evolution that are likely to be encountered in the biological problems we have in mind.

We next consider the same Schnakenberg system on a domain with evolution of the form

\[
A_1(\xi, t) = \left(1 + 2 \sin \left(\frac{\pi t}{T}\right) |\xi|^2\right) \xi_i,
\]

with final time \( T = 1000 \). We select the same parameter values as Table 3, apart from the parameter \( \gamma \) which we set equal to 1. The initial domain (and reference domain) is taken as the square \([-1, 1]^2\]. Figure 4 shows the activator concentrations on a domain with evolution of the form (5.5). We observe the now familiar spot-splitting behaviour as the domain grows and spot-annihilation as the domain contracts. Interestingly, we observe that the spots appear to orient themselves to maintain a relatively uniform level of separation (which is a characteristic of Turing patterns due to their intrinsic wavelength) even with this highly nonlinear form of domain evolution.

Along with 2 component RDSs, 3 component RDSs where a second inhibitor quenches established maxima have been widely studied [22]. Many interesting phenomena, which do not occur in 2 component systems, such as out of phase oscillations and spatiotemporal patterning which does not reach a steady state (even on fixed domains) are observed. The applications of such 3 component systems are of much importance, for example in the modelling of cell polarisation during chemotaxis [21]. To illustrate the versatility of our method in dealing with multiple component systems, we now present results for a three

<table>
<thead>
<tr>
<th>Reaction kinetic parameters</th>
<th>Growth and numerical parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_1 )</td>
<td>( D_2 )</td>
</tr>
<tr>
<td>0.01</td>
<td>1.0</td>
</tr>
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</table>

Table 3. Parameter values for numerical experiments with the Schnakenberg kinetics.
Figure 2. Snapshots of the discrete activator ($u_1$) profile for the Schnakenberg reaction kinetics on a domain with spatially linear evolution at times 0, 580, 1000, 1500 and 2000. The substrate ($u_2$) profile is omitted as they are out of phase with those of the activator. For parameter values see Table 3. The results are computed using the evolving domain formulation (4.11) with a uniform timestep and mesh. We observe the formation of a half spot which reorients to a single spot positioned in the center of the domain. As the domain contracts this single spot is annihilated with the domain at end time exhibiting no patterns.

Figure 3. Snapshots of the discrete activator ($u_1$) profile for the Schnakenberg reaction kinetics on a domain with spatially nonlinear evolution at times 0, 590, 1000, 1750 and 2000. For parameter values see Table 3. The results are computed using the reference domain formulation (4.2) with a uniform timestep and mesh. Although the evolution of the domain boundary is identical to the spatially linear case, the pattern transitions observed are markedly different with the formation of a half spot that splits into two half spots which are annihilated as the domain contracts to leave a final domain with no patterns.
component model. We first consider a fixed domain, to illustrate both the qualitatively different solution behaviour to the 2 component case and that our method is readily applicable to multi-component RDSs posed on fixed domains.

5.5. Definition (Global and local inhibition kinetics [22]). The following model is comprised of a single self-enhancing activator \( u_1 \) antagonised by global (fast diffusing) and local (slow diffusing) inhibitors; \( u_2 \) and \( u_3 \) respectively:

\[
\begin{align*}
  f_1 (u_1, u_2, u_3) &= \gamma \left( \frac{s(u_1^2 + b_1)}{u_2(1 + s_3 u_3)} - r_1 u_1 \right), \\
  f_2 (u_1, u_2, u_3) &= \gamma \left( s u_1^2 - r_2 u_2 \right), \\
  f_3 (u_1, u_2, u_3) &= \gamma \left( r_3 u_1 - r_3 u_3 \right),
\end{align*}
\]

where \( 0 \leq s, b_1, r_1, s_3, r_2, r_3, \gamma, \gamma < \infty \).
We select the set of parameter values given in Tables 4 and 5. We take the domain to be the square

\[
\hat{\Omega} = [-1, 1]^2.
\]

Snapshots of the discrete solutions are reported in Figure 5. An initial 4 spot pattern forms with a rapid transition to a 2 spot solution. The 2 spots then move around the domain boundary in a traveling wave-like fashion. As expected from intuition, the activator \( u_1 \) and local inhibitor \( u_3 \) concentrations are significantly more localized than the global inhibitor concentration \( u_3 \). For details on the behavior of 3 component systems (on fixed domains) and heuristic explanations of the observed behavior we refer to [22]. The behavior is markedly different to the 2-species case. No spatially inhomogeneous steady state is observed. None of the species are in or out of phase with spatial peaks of the global inhibitor travelling slightly ahead of spatial peaks of the activator which travels ahead of the spatial peaks of the local inhibitor.

We now consider the same system posed on an evolving domain. Figure 6 shows snapshots of the evolution on a domain with growth of the form (5.2) and parameter values as given in Tables 4 and 6. Broadly speaking similar behavior to the 2-component case is observed with the patterning mode (number of spots) generally increasing as the domain grows and decreasing as the domain contracts. The initial pattern is a 2 peak pattern that exhibits traveling wave behavior similar to the fixed case. After the domain has grown sufficiently large new peaks appear either via splitting of existing peaks or peak insertion. When multi-peak patterns are present the behavior is much more complicated than the two component case, the peaks travel around the domain and can collide leading to peak-merging or when peaks are in close proximity peak-annihilation, as reported in Figure 7. This behavior of peak-merging and annihilation was observed previously by Venkataraman et al. [32] for 2 component systems, the novelty in the 3 component case is that this behavior is observed even as the domain grows. This is of interest as with this specific 3 component system domain growth (contraction) does not lead to a monotonic increase (decrease) in the number of peaks. Our observations of these novel behaviors of 3 component systems on evolving domains is to the best of our knowledge new and definitely warrants further investigation.

<table>
<thead>
<tr>
<th>( D_1 )</th>
<th>( D_2 )</th>
<th>( D_3 )</th>
<th>( \gamma )</th>
<th>( s )</th>
<th>( s_3 )</th>
<th>( r_1 )</th>
<th>( r_2 )</th>
<th>( r_3 )</th>
<th>( b_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>100</td>
<td>0.01</td>
<td>( 10^4 )</td>
<td>0.005</td>
<td>0.8</td>
<td>0.005</td>
<td>0.008</td>
<td>0.001</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table 4. Parameter values for numerical experiments with the 3 component kinetics.

<table>
<thead>
<tr>
<th>( T )</th>
<th>( \tau )</th>
<th>DOFs</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>( 10^{-3} )</td>
<td>8321</td>
</tr>
</tbody>
</table>

Table 5. Numerical parameter values for experiments with the 3 component kinetics on a fixed domain.

<table>
<thead>
<tr>
<th>( \kappa )</th>
<th>( T )</th>
<th>( \tau )</th>
<th>DOFs</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>100</td>
<td>( 10^{-3} )</td>
<td>8321</td>
</tr>
</tbody>
</table>

Table 6. Parameter values for numerical experiments with the 3 component kinetics on an evolving domain.
Figure 5. Snapshots of the discrete activator $u_1$ (left), discrete global inhibitor $u_2$ (middle) and discrete local inhibitor $u_3$ (right) for the 3 component system (5.6) on a fixed domain at times 0.65, 1, 1.5, 2, 3.5 and 5. The color (grey-scale) legend to the right of each column indicates the numerical range of each component during the experiment. The global inhibitor concentration is less spatially localised than the activator and local inhibitor concentration. We observe travelling wave like solutions. An initial 4 peak solution forms, subsequently 2 peaks are annihilated leaving a 2 peak solution which travels around the boundary of the domain for the remainder of the evolution.
Figure 6. Snapshots of the discrete activator $u_1$ (top), discrete global inhibitor $u_2$ (middle) and discrete local inhibitor $u_3$ (bottom) for the 3 component system (5.6) on a domain with spatially linear evolution at times 0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9 and 10 reading clockwise. The color (grey-scale) legend above each row indicates the numerical range of each component during the experiment. Generally more peaks are observed on larger domains, however the behaviour is much richer than the 2 component case with the travelling wave like nature of the solutions leading to peak collisions which result in spot merging or peak annihilation when spots move into close proximity.
6. Conclusion

We have presented and analysed a fully discrete finite element scheme to approximate the solution to semilinear RDSs posed on continuously evolving domains. Given suitable assumptions on the reaction kinetics and domain evolution we have shown that the proposed scheme converges at an optimal rate in the $L_{\infty}(0, T; L_2(\Omega_t)^m)$ norm. This result constitutes, to the best of our knowledge, one of the first studies of the convergence of a numerical method to approximate the solution to this widely studied class of problems. To illustrate the versatility of the proposed method we have presented examples for 2 and 3 component RDSs on evolving domains. We have observed novel solution behaviour such as patterning that maintains a uniform wavelength on domains with highly nonlinear evolution and spot-annihilation and -merging in 3 component systems on growing domains that results in domain growth having a non-monotonic influence on the patterning mode number.

The computational method considered in this work has applications to the study of biological pattern formation, a field in which computer simulations of RDSs on evolving domains are widespread. The scheme presented provides a practical numerical method that should prove useful to scientists in the field of developmental biology and in other fields where semilinear RDSs are encountered.

The problems we have in mind are inherently posed on long time-scales and involve large spatial deformations. Domain evolution may be viewed as changing the coefficients of the PDE (in the reference framework) or altering the mesh-size of the triangulation (in the evolving framework). Non uniform growth can promote patterning in certain regions of the domain (for example in the simulations on the reference domain in Figure 4 patterning occurs away from the center of the domain, in regions where growth is fast). Moreover, the relatively fast time-scale in which pattern formation occurs necessitates the use of a large number of timesteps to accurately capture the patterning as the domain evolves. Also from our numerical experience the solution behaviour appears to be one of growth induced bifurcations between a series of quasi-steady patterns (in the 2 component case). In light of these considerations, deriving adaptive schemes for the solution of RDSs on evolving domains is of importance and is a focus of our current research. Preliminary results in this respect are presented in [31], where adaptive schemes based on error estimates for the spatial discretisation and error indicators for the temporal discretisation are derived and implemented. We also wish to extend our analysis to the ALE formulation [9] (of which the Eulerian and Lagrangian formulations considered in this study are special cases). This formulation would allow consideration of adaptive moving mesh methods and for suitably chosen time-discretisations has attractive stability properties when domain evolution is nonlinear with respect to space [5,18]. RDSs posed on evolving surfaces or domains with topological changes are becoming increasingly important in applications and extension of the analysis to these scenarios is an important subject for future work.
We also wish to consider cases where domain evolution is unknown or stochastic as these scenarios have applications to cell motility and tumour growth.

REFERENCES


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